Butanoic acid, 2-chloro, 1-methylethyl ester

Inchi: InChI=1S/C7H13ClO2/c1-4-6(8)7(9)10-5(2)3/h5-6H,4H2,1-3H3
InchiKey: DAOWVENIDWCKPM-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCC(Cl)C(=O)OC(C)C
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-242.67	kJ/mol	Joback Method
hf	-458.91	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	43.94	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.955		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	967.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	959.00		NIST Webbook
ripol	1298.00		NIST Webbook
ripol	1291.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1304.00		NIST Webbook
ripol	1327.00		NIST Webbook
tb	472.40	K	Joback Method
tc	663.16	K	Joback Method
tf	240.73	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	265.59	J/mol×K	472.40	Joback Method
cpg	277.03	J/mol×K	504.19	Joback Method
cpg	288.00	J/mol×K	535.99	Joback Method
cpg	298.52	J/mol×K	567.78	Joback Method
cpg	308.57	J/mol×K	599.57	Joback Method
cpg	318.17	J/mol×K	631.37	Joback Method
cpg	327.32	J/mol×K	663.16	Joback Method
dvisc	0.0064287	Pa×s	240.73	Joback Method
dvisc	0.0025878	Pa×s	279.34	Joback Method
dvisc	0.0012993	Pa×s	317.95	Joback Method
dvisc	0.0007574	Pa×s	356.56	Joback Method
dvisc	0.0004906	Pa×s	395.18	Joback Method
dvisc	0.0003433	Pa×s	433.79	Joback Method
dvisc	0.0002547	Pa×s	472.40	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28590&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume